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Nuclear Properties

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Nuclear reactions and nuclear structure play an essential role in the science to be investigated in the Science-Based Stockpile Stewardship Program. In addition, there are nuclear physics applications relying on similar data in Threat Reduction, next-generation nuclear reactors, nuclear astrophysics, and at the Rare Isotope Accelerator (RIA).

Our first challenge is to arrive at a comprehensive and unified description of nuclei and their reactions that is grounded in the interactions between the constituent nucleons. Current phenomenological models of nuclear structure and reactions should be replaced with a well-founded microscopic (e.g. ab-initio) theory that will deliver maximum predictive power with minimal uncertainties that are well quantified. To achieve this goal requires a national effort linking theoretical physics and computational science together to develop forefront software for state-of-the-art architectures. Our second challenge applies to heavy nuclei, such as actinides, where truly ab-initio methods are still beyond our reach: This challenge is to develop more rigorous and predictive theories for fission, and radiative capture, and use a rigorous validation methodology to demonstrate the improved predictive capability.

A national capability to calculate nuclear structure and low-energy nuclear cross sections (and to assess their uncertainties) will require the development of a multi-pronged program of theoretical, algorithmic, and computational improvements that will utilize leadership-class computation to solve several long-standing fundamental problems in nuclear physics, and will deliver nuclear cross section information critical to DOE programs that is more accurate than is currently available. DOE needs this capability because in many instances experimental data are not available or obtainable even with the construction of advanced exotic beam facilities. Thus, a reliance on theory or extrapolations from known data is required in order to make predictions. An expansion of the computational techniques and methods currently employed, and developments of new treatments, will be necessary to take advantage of petascale architectures and to demonstrate the capability of the leadership class machines to deliver new science heretofore impossible. The effort would entail both improving the predictive power of nuclear calculations by connecting microscopic effective interactions to the basic nuclear interactions, and assessing quantitative error estimates of the results.

The need to develop better theory for the description of nuclear structure and reaction cross sections for various applications has been pointed out in several high-level documents including the Nuclear Science Advisory Committee (NSAC) 2004 Report: *A*

Vision for Nuclear Theory; the NSAC 2005 Report: *Guidance for Implementing the 2002 Long-Range Plan*; and the DOE *Path to Sustainable Nuclear Energy* (2005), which points to the need for cross sections in planning for the advanced reactor technology. During the past 10 years, the nuclear theory community has been pursuing developments of sophisticated computational techniques to investigate properties of nuclei based only on the underlying nuclear forces. These developments have led to a new understanding of light nuclei using ab-initio many-body methods, and of heavier nuclei using self-consistent mean-field techniques. Furthermore, the first steps have been taken to understand nuclear reactions using ab-initio techniques.

Nuclear reactions involving fission to date are modeled in a semi-phenomenological way. In part this is because of the extreme sensitivity of the calculated fission cross section to nuclear structure properties such as fission barriers and nuclear level densities, at various nuclear deformations. However many applications, including advanced reactors and fuel cycles, need more accurate predictions of fission cross sections for shorter lived unstable species where few reliable measurements exist. We need more advanced theories for fission, combined with nuclear reaction theories that utilize these advances (including possible dynamical effects), to predict fission cross sections for unstable actinide species. A deeper understanding is also needed for post-scission fission physics, regarding our understanding of the energy spectrum of emitted fission neutrons and gamma-rays, and fission fragment distributions. The significant challenge for the community here is to demonstrate increased predictive power for a new fission theory, i.e. not just to develop more sophisticated fission theories, but to demonstrate through a more rigorous validation process that such a new theory indeed has an increased predictive capability for fission cross sections.

We also need to have more precise predictions of radiative neutron capture cross sections in the keV-MeV region. Capture is notoriously difficult to predict theoretically. However, a wide range of applications (s and r-process nucleosynthesis, advanced reactors and transmutation technologies, as well as NNSA applications) need more accurate theoretical methods to extrapolate from measured on-stability regions to off-stability regions that are important in these extreme environments. We should emphasize, though, that improved capture cross sections are also needed for stable targets, because of historical difficulties in precise measurements. Thus, in the higher energy region (400 keV-1 MeV, say) few reliable measurements exist, and methods – both theoretical, and phenomenological methods tied to measurements – are needed to more accurately determine these capture cross sections. Advance reactor technologies need such data for the actinides.

We need to understand neutron cross sections, nuclear decay, and fission on many nuclei ranging from light to heavy systems. Calculation of neutron cross sections requires a detailed knowledge of nuclear properties. Theoretical error estimates for cross sections will be relevant to covariance studies for various evaluations.

Examples of specific research areas include:

- calculate light nuclear structure and reaction information using realistic nuclear potentials,
- describe medium mass and heavy nuclei with nuclear density functional theory and its extensions,
- incorporate new density functional information into reaction cross section calculations including the building of theoretically based optical potentials,
- develop a robust computational description of nuclear level densities,
- develop improved theories of nuclear fission and capture
- integrate mathematical algorithms with science applications for optimal performance, and
- deliver to the community open-source software for the calculation of nuclear cross sections relevant to the various DOE missions.

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